



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:33 PM GMT

PDB ID : 4IPE
Title : Crystal structure of mitochondrial Hsp90 (TRAP1) with AMPPNP
Authors : Partridge, J.R.; Lavery, L.A.; Agard, D.A.
Deposited on : 2013-01-09
Resolution : 2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

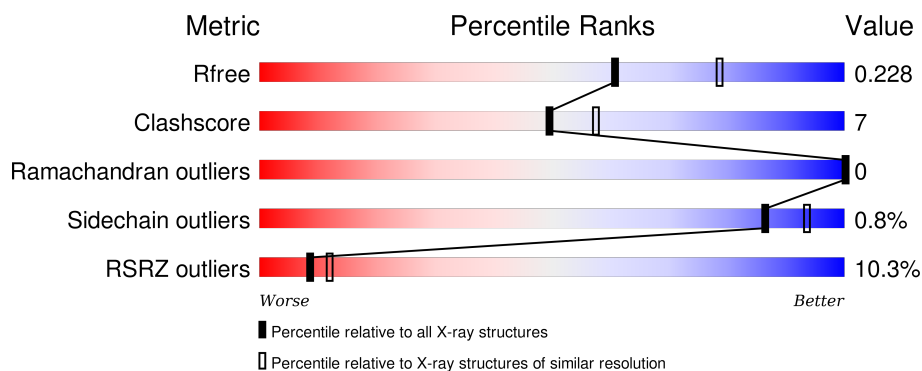
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	719	<div> <div>9%</div> <div>67%</div> <div>14%</div> <div>18%</div> </div>
1	B	719	<div> <div>8%</div> <div>71%</div> <div>12%</div> <div>16%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	1	0
			4720	2991	816	891	22			
1	B	601	Total	C	N	O	S	0	3	0
			4872	3092	841	917	22			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Co 2 2	0	0
4	A	2	Total Co 2 2	0	0

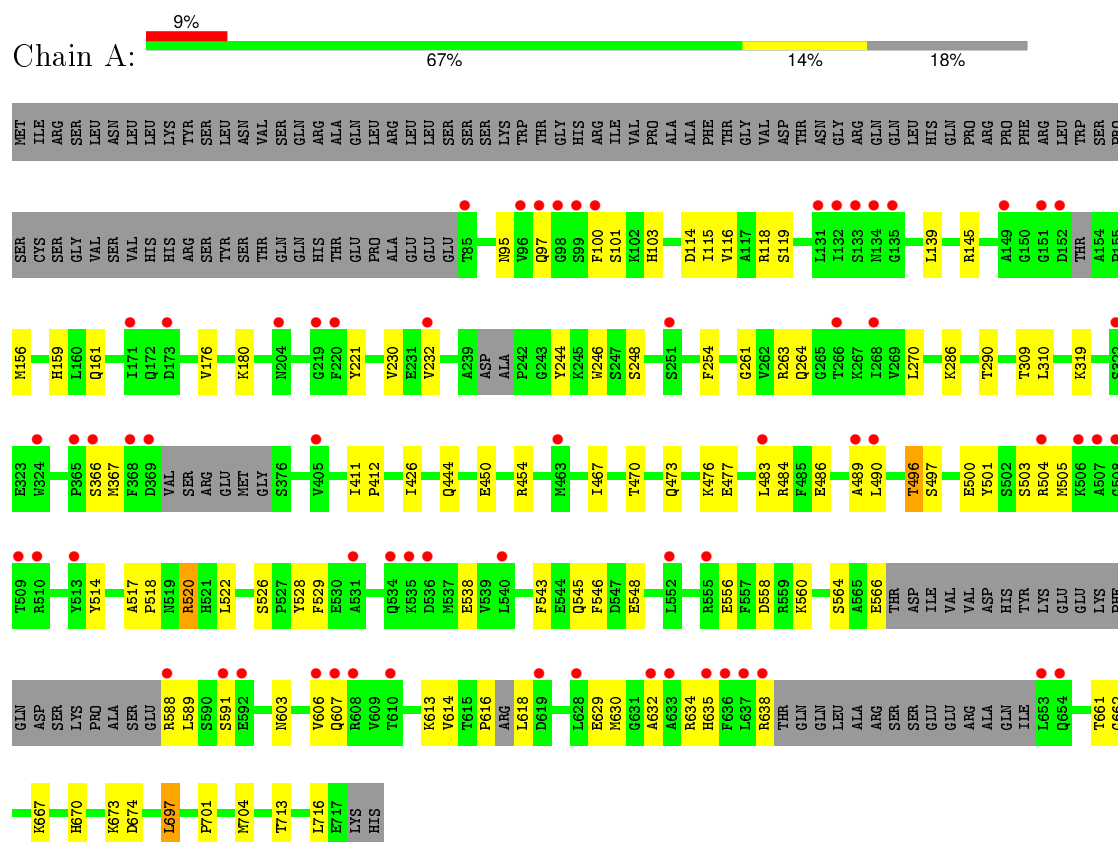
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	132	Total O 132 132	0	0
5	B	148	Total O 148 148	0	0

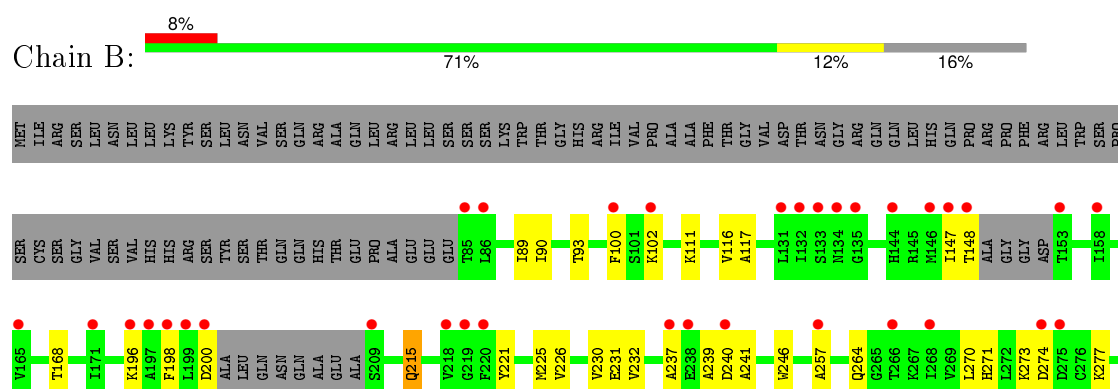
3 Residue-property plots

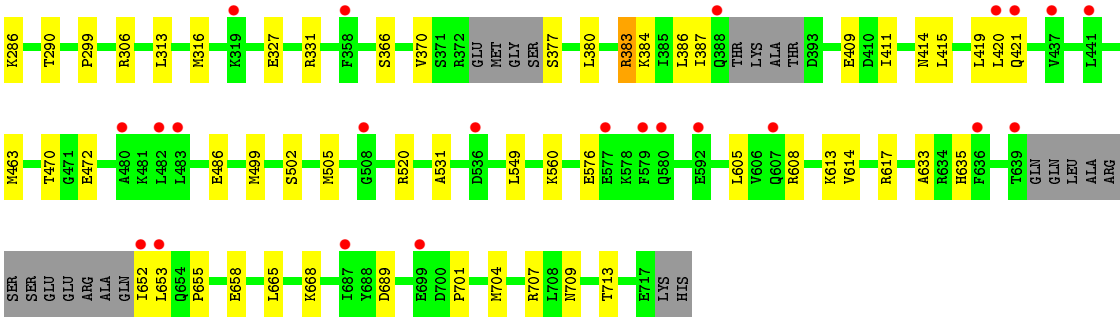
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: TNF receptor-associated protein 1



- Molecule 1: TNF receptor-associated protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.98 Å 96.36 Å 125.15 Å 90.00° 134.34° 90.00°	Depositor
Resolution (Å)	26.24 – 2.29 26.55 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (26.24-2.29) 92.1 (26.55-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1214)	Depositor
R, R_{free}	0.180 , 0.225 0.183 , 0.228	Depositor DCC
R_{free} test set	1883 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.005 for h,-k,-h-l 0.015 for -h-2*l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67286 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9940	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, MG, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/4806	0.59	1/6473 (0.0%)
1	B	0.42	0/4970	0.58	1/6695 (0.0%)
All	All	0.41	0/9776	0.59	2/13168 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	GLY	N-CA-C	-7.71	93.83	113.10
1	B	215	GLN	N-CA-CB	-5.66	100.41	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4720	0	4720	71	0
1	B	4872	0	4882	74	0
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	132	0	0	1	0
5	B	148	0	0	7	0
All	All	9940	0	9628	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:CG2	1:B:420:LEU:HD22	1.63	1.28
1:B:411:ILE:HG21	1:B:420:LEU:HD22	1.15	1.08
1:B:240:ASP:H	1:B:241:ALA:HB2	1.32	0.94
1:A:588:ARG:HD3	1:A:662:GLY:HA3	1.51	0.91
1:B:411:ILE:HG21	1:B:420:LEU:CD2	2.05	0.84
1:B:411:ILE:HG22	1:B:420:LEU:HD22	1.58	0.83
1:A:505:MET:SD	1:A:560:LYS:NZ	2.50	0.83
1:B:147:ILE:H	1:B:148:THR:HA	1.43	0.81
1:A:588:ARG:HD3	1:A:662:GLY:CA	2.12	0.79
1:A:119:SER:HA	1:B:421:GLN:HE22	1.49	0.77
1:A:716:LEU:O	1:B:668:LYS:NZ	2.20	0.73
1:B:377:SER:N	5:B:1004:HOH:O	2.21	0.73
1:A:116:VAL:HG11	1:A:221:TYR:HB2	1.73	0.70
1:B:116:VAL:HG11	1:B:221:TYR:HB2	1.73	0.70
1:A:616:PRO:O	1:A:618:LEU:N	2.25	0.70
1:B:383:ARG:HH21	1:B:409:GLU:HG2	1.57	0.68
1:A:101:SER:OG	1:A:103:HIS:NE2	2.21	0.67
1:B:232:VAL:HB	1:B:246:TRP:HB3	1.76	0.67
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.77	0.67
1:B:414:ASN:ND2	1:B:419:LEU:HB2	2.11	0.66
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.27	0.65
1:B:701:PRO:O	1:B:704:MET:HG2	1.98	0.64
1:B:531:ALA:O	1:B:617:ARG:NH2	2.31	0.63
1:A:119:SER:O	1:B:415:LEU:N	2.32	0.62
1:B:499:MET:HG2	5:B:1016:HOH:O	2.00	0.62
1:B:327:GLU:OE1	1:B:331:ARG:NH2	2.33	0.61
1:B:414:ASN:ND2	1:B:419:LEU:HD12	2.17	0.60
1:A:486:GLU:OE1	1:A:520:ARG:NH1	2.35	0.60
1:B:605:LEU:HD23	1:B:608:ARG:HH21	1.69	0.58
1:B:414:ASN:HD22	1:B:419:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:OG	1:A:367:MET:N	2.38	0.57
1:B:709:ASN:O	1:B:713:THR:HG23	2.05	0.57
1:B:168:THR:HG22	5:B:954:HOH:O	2.05	0.57
1:A:606:VAL:HG12	1:A:607:GLN:HG3	1.87	0.57
1:A:100:PHE:HB3	1:B:257:ALA:HB2	1.86	0.56
1:B:117:ALA:O	1:B:225:MET:HG2	2.06	0.56
1:A:139:LEU:HD22	1:A:156:MET:HB3	1.88	0.55
1:A:114:ASP:OD2	1:A:118:ARG:NH2	2.41	0.55
1:A:558:ASP:O	1:A:560:LYS:HG3	2.07	0.54
1:B:502:SER:HA	1:B:505:MET:HE3	1.90	0.54
1:A:489:ALA:CB	1:A:538:GLU:HG3	2.37	0.54
1:A:309:THR:O	1:A:309:THR:HG22	2.07	0.54
1:A:518:PRO:HD2	1:A:630:MET:HE2	1.90	0.54
1:B:239:ALA:H	1:B:241:ALA:HB2	1.73	0.54
1:B:313:LEU:HA	1:B:316:MET:HE2	1.88	0.53
1:A:232:VAL:HB	1:A:246:TRP:HB3	1.90	0.53
1:A:263:ARG:NH1	5:A:997:HOH:O	2.36	0.53
1:A:319:LYS:H	1:A:319:LYS:HE2	1.74	0.52
1:B:240:ASP:N	1:B:241:ALA:HB2	2.13	0.52
1:B:274:ASP:HA	1:B:277:LYS:HE3	1.91	0.52
1:B:502:SER:HA	1:B:505:MET:CE	2.39	0.52
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.91	0.51
1:B:470:THR:HG22	1:B:472:GLU:H	1.75	0.51
1:B:380:LEU:HD13	1:B:420:LEU:HD11	1.92	0.51
1:B:383:ARG:O	1:B:384:LYS:HB2	2.11	0.51
1:B:652:ILE:N	5:B:999:HOH:O	2.44	0.50
1:B:240:ASP:HB2	1:B:241:ALA:HA	1.94	0.50
1:B:633:ALA:HB1	1:B:653:LEU:HD11	1.94	0.49
1:B:652:ILE:HG22	1:B:653:LEU:N	2.27	0.49
1:B:380:LEU:CD1	1:B:420:LEU:HD11	2.43	0.49
1:B:147:ILE:N	1:B:148:THR:HA	2.11	0.49
1:B:198:PHE:O	1:B:200:ASP:HA	2.12	0.49
1:A:501:TYR:O	1:A:505:MET:HG3	2.12	0.49
1:B:230:VAL:HG22	1:B:270:LEU:HD22	1.94	0.49
1:B:237:ALA:HB2	1:B:264:GLN:HE22	1.77	0.48
1:A:286:LYS:O	1:A:290:THR:HG23	2.13	0.48
1:A:450:GLU:HG3	1:A:454:ARG:HH21	1.78	0.48
1:B:226:VAL:O	1:B:273:LYS:HG2	2.13	0.48
1:B:100:PHE:CE1	1:B:102:LYS:HE3	2.49	0.47
1:A:713:THR:HG22	1:B:665:LEU:HB2	1.95	0.47
1:A:489:ALA:HB2	1:A:538:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PRO:HD2	1:A:630:MET:CE	2.45	0.47
1:B:689:ASP:OD2	1:B:707:ARG:NH2	2.43	0.47
1:A:483:LEU:O	1:A:484:ARG:HD3	2.14	0.47
1:A:119:SER:CA	1:B:421:GLN:HE22	2.24	0.46
1:A:522:LEU:HD11	1:A:697:LEU:HD13	1.97	0.46
1:B:100:PHE:HE1	1:B:102:LYS:HE3	1.80	0.46
1:B:411:ILE:HG22	1:B:420:LEU:CD2	2.38	0.46
1:A:588:ARG:HD3	1:A:662:GLY:HA2	1.96	0.46
1:B:605:LEU:HD23	1:B:608:ARG:NH2	2.29	0.46
1:B:237:ALA:HB2	1:B:264:GLN:NE2	2.30	0.46
1:B:505:MET:HE1	1:B:560:LYS:HD3	1.98	0.46
1:A:528:TYR:CD1	1:A:566:GLU:HA	2.51	0.46
1:A:248:SER:HB2	1:A:254:PHE:HB3	1.97	0.46
1:B:111:LYS:NZ	5:B:1041:HOH:O	2.48	0.46
1:A:470:THR:O	1:A:476:LYS:HE3	2.16	0.46
1:A:500:GLU:O	1:A:503:SER:HB3	2.16	0.46
1:A:548:GLU:OE1	1:A:634:ARG:NH1	2.49	0.46
1:A:591:SER:OG	1:A:591:SER:O	2.34	0.45
1:A:500:GLU:O	1:A:504:ARG:HG3	2.16	0.45
1:B:411:ILE:CG2	1:B:420:LEU:CD2	2.60	0.45
1:A:634:ARG:HB3	1:A:638:ARG:HH21	1.82	0.45
1:B:286:LYS:O	1:B:290:THR:HG23	2.16	0.45
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.52	0.45
1:A:603:ASN:O	1:A:606:VAL:HG23	2.17	0.45
1:A:613:LYS:HG2	1:A:614:VAL:H	1.81	0.45
1:A:145:ARG:HE	1:A:176:VAL:HG21	1.82	0.44
1:B:386:LEU:HD11	5:B:1048:HOH:O	2.17	0.44
1:A:526:SER:HB3	1:A:529:PHE:HB3	2.00	0.44
1:B:653:LEU:C	1:B:655:PRO:HD3	2.37	0.44
1:A:514:TYR:CE1	1:A:564:SER:HB3	2.53	0.44
1:B:486:GLU:OE1	1:B:520:ARG:HD3	2.17	0.44
1:A:517:ALA:O	1:A:543:PHE:HA	2.17	0.44
1:A:566:GLU:OE2	1:A:629:GLU:HA	2.18	0.44
1:A:564:SER:O	1:A:566:GLU:N	2.51	0.44
1:A:497:SER:OG	1:A:500:GLU:HG3	2.18	0.43
1:A:632:ALA:O	1:A:635:HIS:N	2.51	0.43
1:B:196:LYS:NZ	1:B:215:GLN:HA	2.32	0.43
1:B:633:ALA:HB1	1:B:653:LEU:CD1	2.48	0.43
1:B:386:LEU:O	1:B:387:ILE:HD13	2.18	0.43
1:B:652:ILE:O	1:B:653:LEU:HG	2.19	0.43
1:A:670:HIS:O	1:A:673:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:HG2	1:A:546:PHE:CD2	2.54	0.42
1:A:263:ARG:HG2	1:A:264:GLN:N	2.35	0.42
1:A:467:ILE:O	1:A:476:LYS:HE2	2.19	0.42
1:B:549:LEU:HD13	1:B:635:HIS:CE1	2.55	0.42
1:B:299:PRO:HB3	1:B:306:ARG:CZ	2.49	0.42
1:B:576:GLU:N	1:B:576:GLU:OE2	2.53	0.42
1:A:589:LEU:HB3	1:A:661:THR:HB	2.01	0.42
1:A:95:ASN:O	1:A:97:GLN:HG2	2.20	0.42
1:A:489:ALA:HB3	1:A:538:GLU:HG3	2.02	0.41
1:A:412:PRO:HD2	1:A:426:ILE:HD11	2.01	0.41
1:A:473:GLN:NE2	1:A:556:GLU:O	2.53	0.41
1:B:331:ARG:HD2	5:B:1017:HOH:O	2.20	0.41
1:A:473:GLN:O	1:A:477:GLU:HG3	2.21	0.41
1:B:613:LYS:O	1:B:658:GLU:HA	2.19	0.41
1:A:159:HIS:CE1	1:B:89:ILE:HD13	2.56	0.41
1:A:701:PRO:O	1:A:704:MET:HG2	2.21	0.41
1:A:490:LEU:HD11	1:A:496:THR:HG21	2.03	0.41
1:A:115:ILE:CG2	1:B:415:LEU:HD22	2.50	0.41
1:A:673:LYS:NZ	1:A:674:ASP:OD2	2.47	0.41
1:A:411:ILE:HA	1:A:412:PRO:HD3	1.90	0.40
1:A:161:GLN:HB2	1:B:90:ILE:HD12	2.03	0.40
1:B:366:SER:O	1:B:370:VAL:HG23	2.21	0.40
1:B:505:MET:HE1	1:B:560:LYS:CD	2.52	0.40
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	575/719 (80%)	545 (95%)	30 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	592/719 (82%)	568 (96%)	24 (4%)	0	100	100
All	All	1167/1438 (81%)	1113 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/634 (81%)	512 (99%)	4 (1%)	86	93
1	B	537/634 (85%)	533 (99%)	4 (1%)	88	94
All	All	1053/1268 (83%)	1045 (99%)	8 (1%)	86	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	A	496	THR
1	A	520	ARG
1	A	697	LEU
1	B	93	THR
1	B	383	ARG
1	B	463	MET
1	B	614	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	421	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ANP	A	801	3	27,33,33	1.37	3 (11%)	30,52,52	0.83	1 (3%)
2	ANP	B	802	3	27,33,33	1.34	5 (18%)	30,52,52	1.04	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	A	801	3	-	0/12/38/38	0/3/3/3
2	ANP	B	802	3	-	0/12/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	ANP	PB-O3A	-2.20	1.56	1.59
2	B	802	ANP	PB-N3B	2.02	1.68	1.63
2	A	801	ANP	PG-N3B	2.65	1.70	1.63
2	B	802	ANP	PG-N3B	2.83	1.70	1.63
2	B	802	ANP	PB-O1B	3.29	1.49	1.46
2	B	802	ANP	PG-O1G	3.49	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PB-O1B	3.60	1.50	1.46
2	A	801	ANP	PG-O1G	4.17	1.50	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	ANP	O1G-PG-N3B	-2.72	107.72	111.90
2	A	801	ANP	PA-O3A-PB	-2.53	124.17	132.67
2	B	802	ANP	O2G-PG-O1G	-2.40	107.11	113.49
2	B	802	ANP	PA-O3A-PB	-2.21	125.24	132.67
2	B	802	ANP	O1B-PB-N3B	-2.03	108.79	111.90
2	B	802	ANP	O3A-PB-N3B	2.27	112.67	106.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	588/719 (81%)	0.48	65 (11%) 7 10	38, 71, 126, 186	0
1	B	601/719 (83%)	0.36	57 (9%) 10 14	40, 66, 108, 145	0
All	All	1189/1438 (82%)	0.42	122 (10%) 9 12	38, 68, 119, 186	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	10.2
1	B	607	GLN	7.2
1	A	508	GLY	7.0
1	B	652	ILE	7.0
1	A	588	ARG	6.7
1	A	607	GLN	6.6
1	A	534	GLN	6.3
1	A	152	ASP	5.2
1	A	96	VAL	5.2
1	A	535	LYS	5.1
1	B	131	LEU	5.1
1	B	653	LEU	5.0
1	A	507	ALA	5.0
1	B	198	PHE	4.8
1	B	146	MET	4.7
1	B	482	LEU	4.7
1	B	420	LEU	4.6
1	A	628	LEU	4.6
1	A	636	PHE	4.5
1	A	368	PHE	4.5
1	A	608	ARG	4.5
1	B	147	ILE	4.4
1	A	638	ARG	4.3
1	A	171	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	268	ILE	4.2
1	A	131	LEU	4.1
1	B	238	GLU	4.1
1	B	86	LEU	4.1
1	A	100	PHE	4.1
1	B	577	GLU	4.0
1	A	632	ALA	3.9
1	A	266	THR	3.9
1	B	421	GLN	3.8
1	A	635	HIS	3.8
1	B	639	THR	3.8
1	A	268	ILE	3.8
1	A	510	ARG	3.8
1	A	531	ALA	3.8
1	B	85	THR	3.7
1	B	257	ALA	3.7
1	A	324	TRP	3.6
1	B	220	PHE	3.5
1	B	153	THR	3.4
1	A	592	GLU	3.4
1	B	199	LEU	3.4
1	A	132	ILE	3.4
1	B	165	VAL	3.4
1	A	85	THR	3.4
1	B	171	ILE	3.4
1	B	148	THR	3.3
1	A	369	ASP	3.3
1	A	99	SER	3.3
1	A	220	PHE	3.2
1	B	135	GLY	3.2
1	B	196	LYS	3.2
1	B	209	SER	3.2
1	A	506	LYS	3.2
1	A	97	GLN	3.1
1	A	619	ASP	3.1
1	B	144	HIS	2.9
1	A	509	THR	2.9
1	A	637	LEU	2.9
1	A	366	SER	2.9
1	A	232	VAL	2.9
1	B	100	PHE	2.8
1	B	441	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	322	SER	2.8
1	A	591	SER	2.8
1	B	200	ASP	2.8
1	B	699	GLU	2.8
1	B	237	ALA	2.8
1	B	437	VAL	2.7
1	A	653	LEU	2.7
1	B	197	ALA	2.7
1	A	540	LEU	2.6
1	A	151	GLY	2.6
1	B	219	GLY	2.6
1	A	365	PRO	2.6
1	A	489	ALA	2.6
1	A	555	ARG	2.6
1	A	133	SER	2.5
1	A	204	ASN	2.5
1	A	610	THR	2.5
1	A	149	ALA	2.5
1	A	483	LEU	2.5
1	B	536	ASP	2.5
1	B	134	ASN	2.5
1	B	358	PHE	2.5
1	A	513	TYR	2.5
1	B	483	LEU	2.5
1	A	134	ASN	2.5
1	B	579	PHE	2.5
1	B	158	ILE	2.5
1	B	275	ASP	2.4
1	A	552	LEU	2.4
1	B	274	ASP	2.4
1	B	636	PHE	2.4
1	A	405	VAL	2.4
1	A	606	VAL	2.4
1	B	580	GLN	2.4
1	A	135	GLY	2.3
1	B	132	ILE	2.3
1	A	504	ARG	2.3
1	B	592	GLU	2.3
1	B	266	THR	2.2
1	B	240	ASP	2.2
1	A	654	GLN	2.2
1	B	218	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	687	ILE	2.2
1	B	388	GLN	2.2
1	B	480	ALA	2.2
1	A	633	ALA	2.1
1	A	98	GLY	2.1
1	B	102	LYS	2.1
1	A	463	MET	2.1
1	A	219	GLY	2.1
1	A	251	SER	2.1
1	B	508	GLY	2.0
1	B	319	LYS	2.0
1	A	173	ASP	2.0
1	A	490	LEU	2.0
1	B	133	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ANP	B	802	31/31	0.98	0.21	0.11	47,54,60,62	0
2	ANP	A	801	31/31	0.99	0.20	-0.01	35,43,48,52	0
3	MG	A	802	1/1	0.89	0.20	-1.15	42,42,42,42	0
3	MG	B	803	1/1	0.96	0.17	-1.48	53,53,53,53	0
4	CO	B	801	1/1	0.98	0.09	-	89,89,89,89	0
4	CO	A	804	1/1	0.87	0.06	-	88,88,88,88	1
4	CO	A	803	1/1	0.89	0.04	-	127,127,127,127	0
4	CO	B	804	1/1	0.71	0.14	-	99,99,99,99	1

6.5 Other polymers

There are no such residues in this entry.